Connecting the evolution and coalescence of 3-dimensional grain structures to reactor-scale phenomena

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We have created a finite-element based, multiple level-set code to model the evolution and coalescence of grains and atomic scale islands during thin film growth. The structure of polycrystalline materials have significant performance implications for microelectronic interconnects, so it is important that modelers have the ability to represent both the structure and evolution of detailed thin film microstructures under processing conditions. Our software tool can simulate the evolution of N grains or atomic-scale proto-grains in 2D or 3D. Grain boundaries are represented implicitly by a set of N+1 scalar fields, $\varphi_i(\mathbf{r}, t)$ expressed on an unstructured mesh, subject to the condition that $\varphi_i(\mathbf{r},t) = 0$ for all $\mathbf{r}$ on the boundary of grain i at time t. This "level set" representation was pioneered by Sethian and Osher [1,2] and avoids many of the difficulties of explicit interface representations. By extracting the zero contour, we can recover the grain boundaries at any time. Because each region is associated with its own scalar field, properties of that region, such as the orientation of the atomic lattice, can be easily retained on a grain-by-grain basis.

The evolution of each grain is computed separately using the usual equation, $\varphi_t + F|\nabla\varphi| = 0$ where F is a speed function that corresponds to the speed of the interface in the direction normal to the interface [1]. We calculate $\nabla\varphi$ using either an explicit Petrov-Galerkin formulation or a positive coefficient scheme [3]. Interactions between level sets representing different regions are then reconciled to bring the various level sets into agreement [4].

Significant distortions in the level sets fields far from the zero levels can occur after several time steps. To address this issue, our code implements a "redistancing" algorithm that corrects these distortions. This redistancing step stablizes the evolution, allowing for simulations that include the coalescense of proto-grains and islands into complex grain structures.

Demonstration of this code are presented, including application within a multiscale framework. Reactor scale simulations of fluid flow and reactant transport are performed, using PHASTA, a finite element based parallel mass and momentum transport code. These reactor scale simulations of simple deposition processes receive reactant consumption data passed to them from the grain-scale in the form of boundary conditions. This allows us to establish concentration fields of reactant both on the scale of tens of centimeters, and using local refinement, on the sub-millimeter scale (Figure 1). In turn, the reactor-scale simulation passes reaction conditions back down to a grain-scale level set simulation. This allows us to show the interaction of phenomena such as reactor-scale reactant depletion on the resulting grain structure.

REFERENCES

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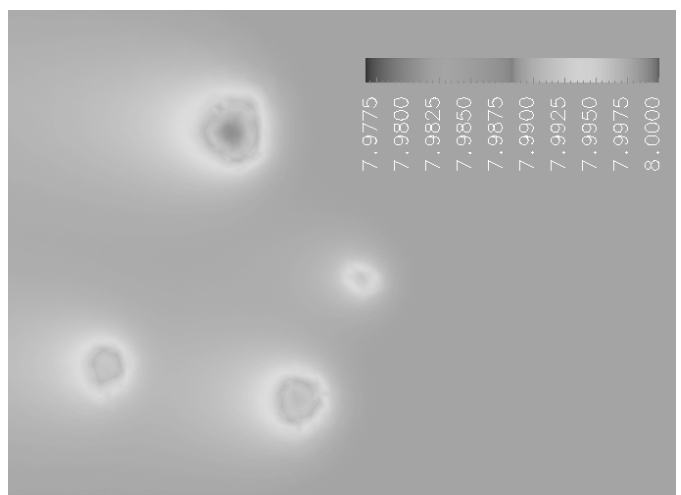
Figure 1. Concentration of Cu^{2+} in the electrolyte over a 200 mm wafer during electrochemical deposition of copper. The small regions (~0.6 mm diameter) shown are areas of depleted reactant over areas where growth has been nucleated. Concentration are given in mmol/liter.